Supporting Information

Catalytic chemodosimeteric approach for detection of nanomolar cyanide ions in water, blood serum and live cell imaging

Rahul Kumar[a], Sana Sandhu[a], Geeta Hundal[a], Vanita Vanita,[b] Amandeep Walia,[b] Prabhpreet Singh[a], and Subodh Kumar[a] *

Corresponding author. Address: Department of Chemistry, UGC Centre for Advanced Studies, Guru Nanak Dev University, Amritsar 143 005, India.

Corresponding author. Mobile: +91 9872361528.

E-mail address: subodh_gndu@yahoo.com

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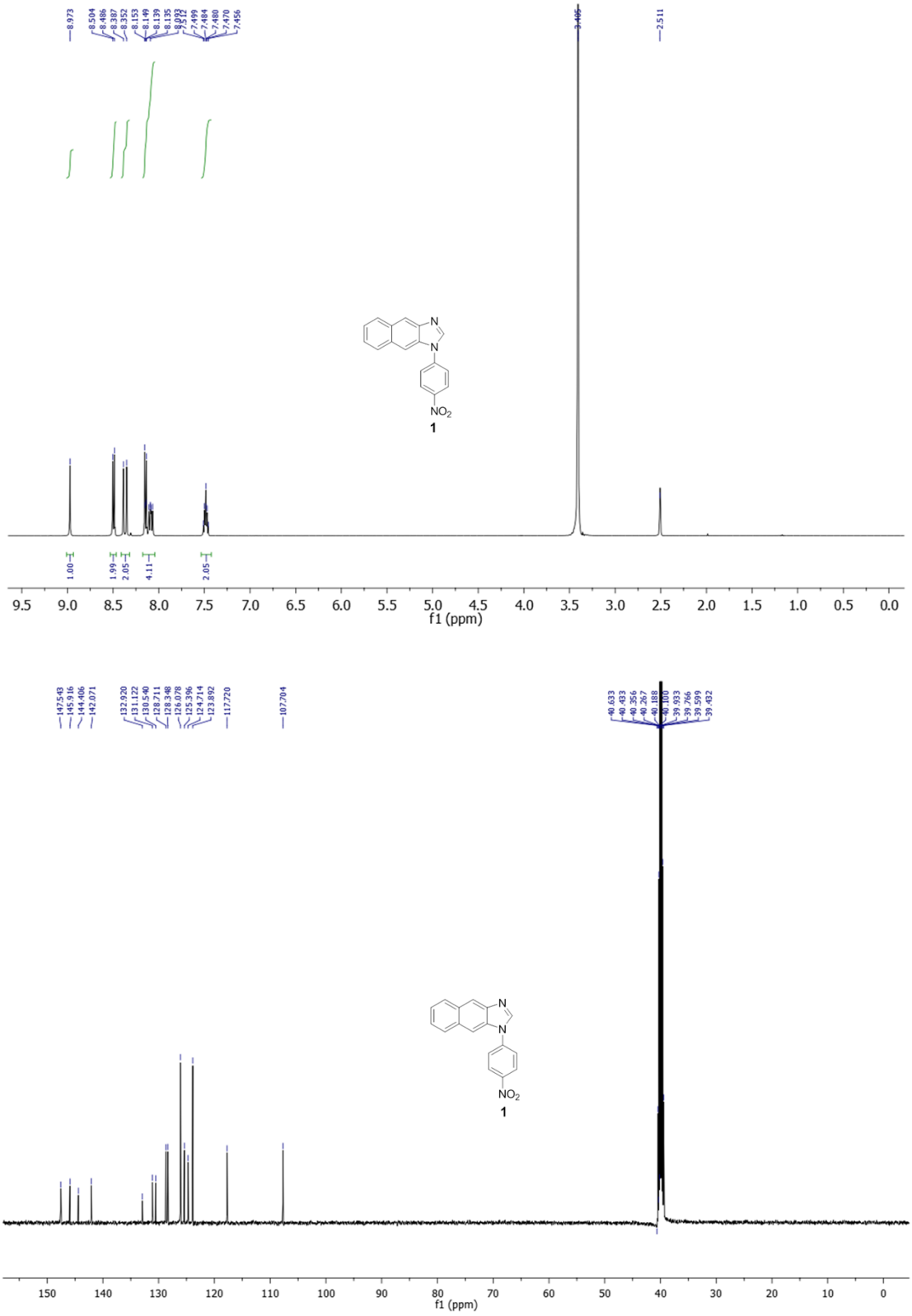


Figure SI 1. ^{1}H and ^{13}C NMR spectra of compound **1**

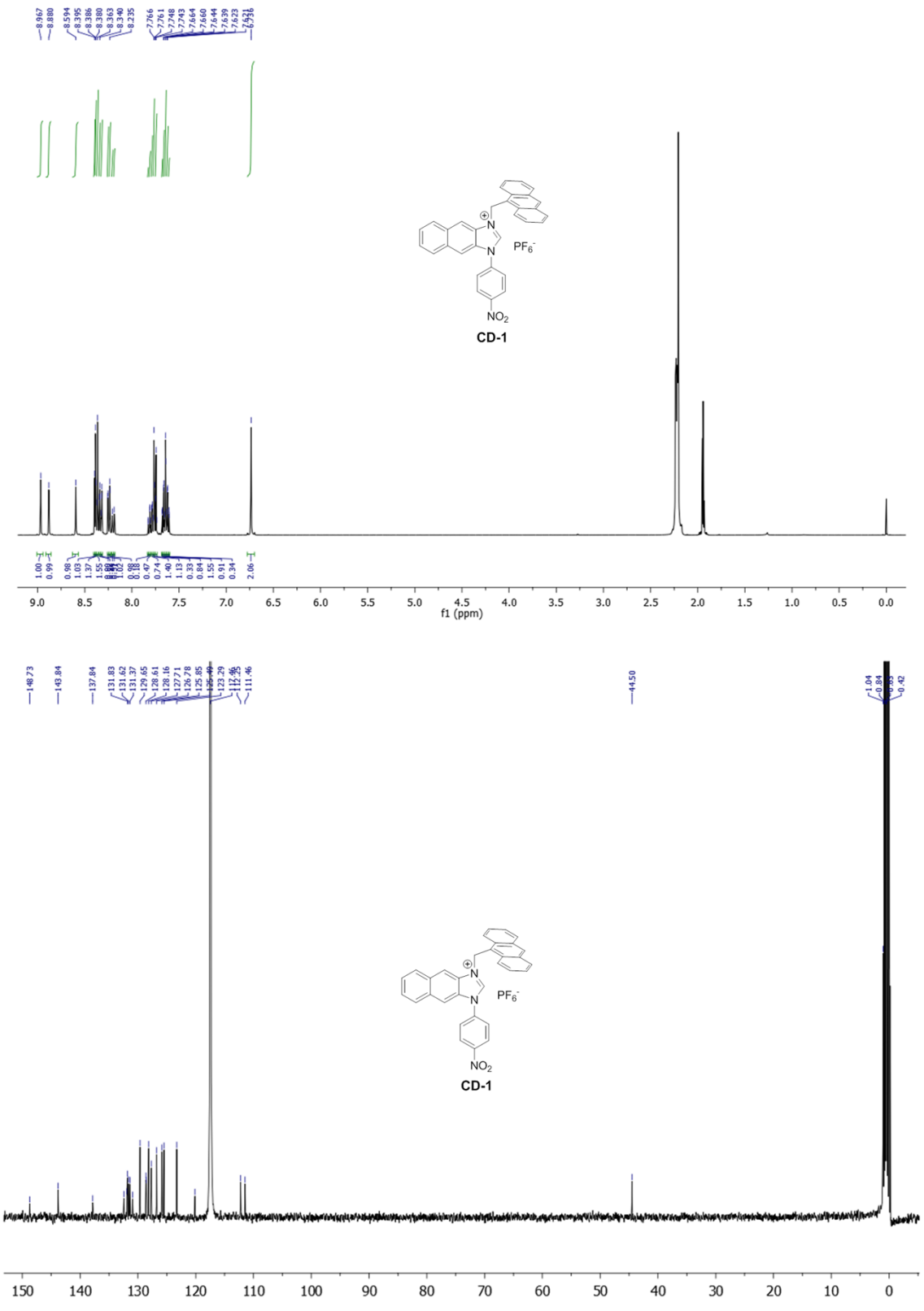


Figure SI 2. ^{1}H and ^{13}C NMR spectra of chemodosimeter **CD-1**

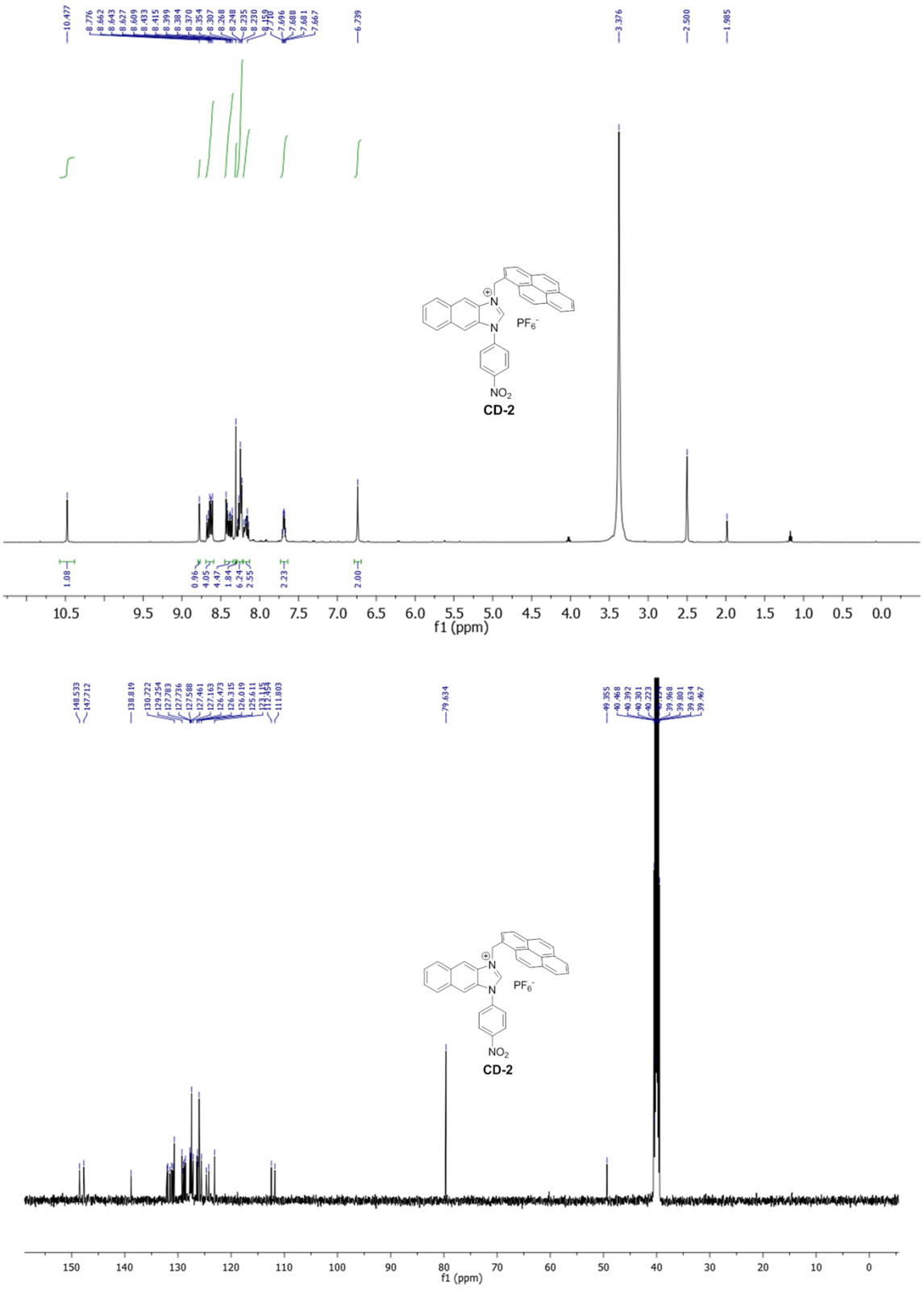


Figure SI 3. ^{1}H and ^{13}C NMR spectra of chemodosimeter **CD-2**

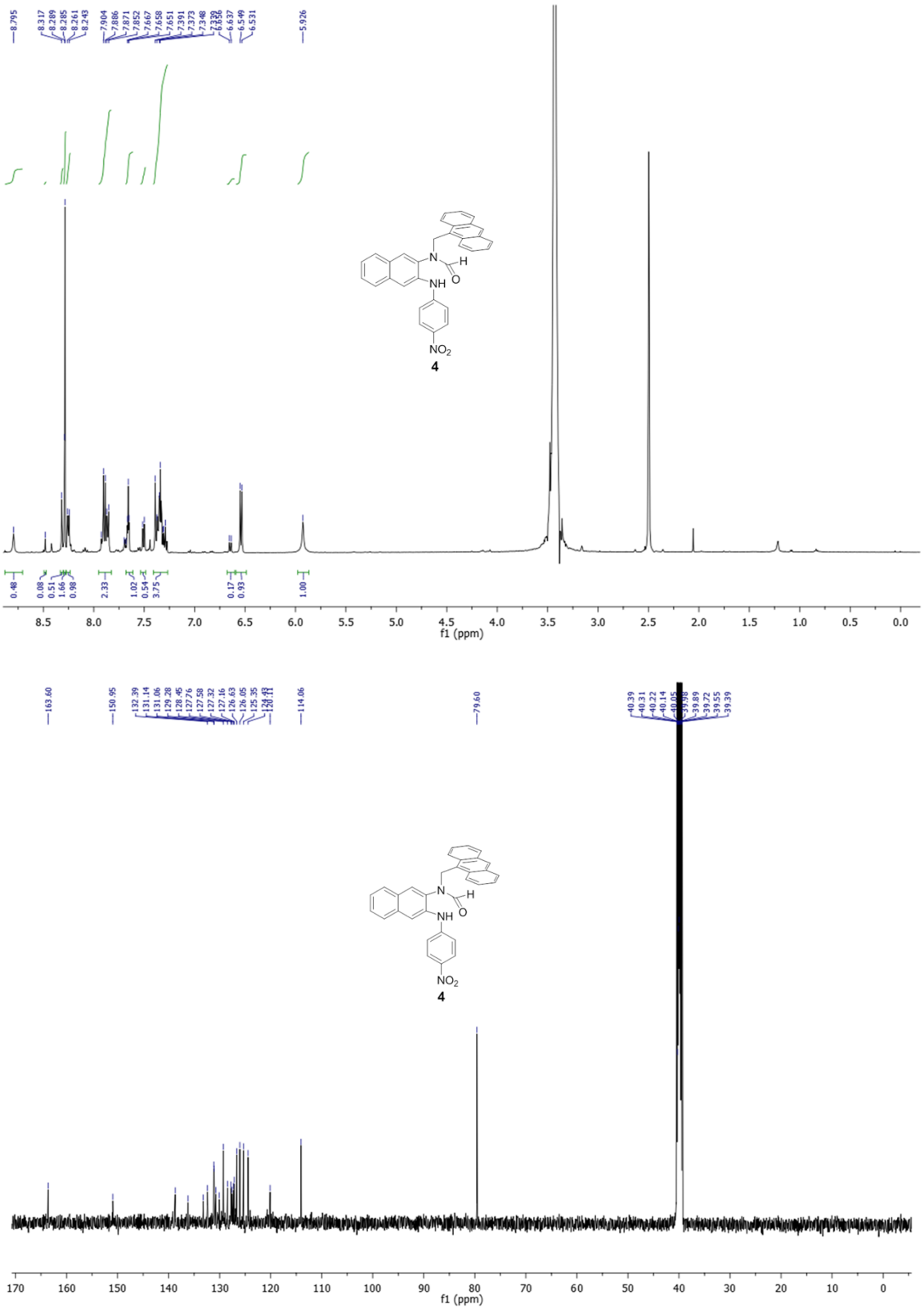


Figure SI 4. ^{1}H and ^{13}C NMR spectra of compound **4**

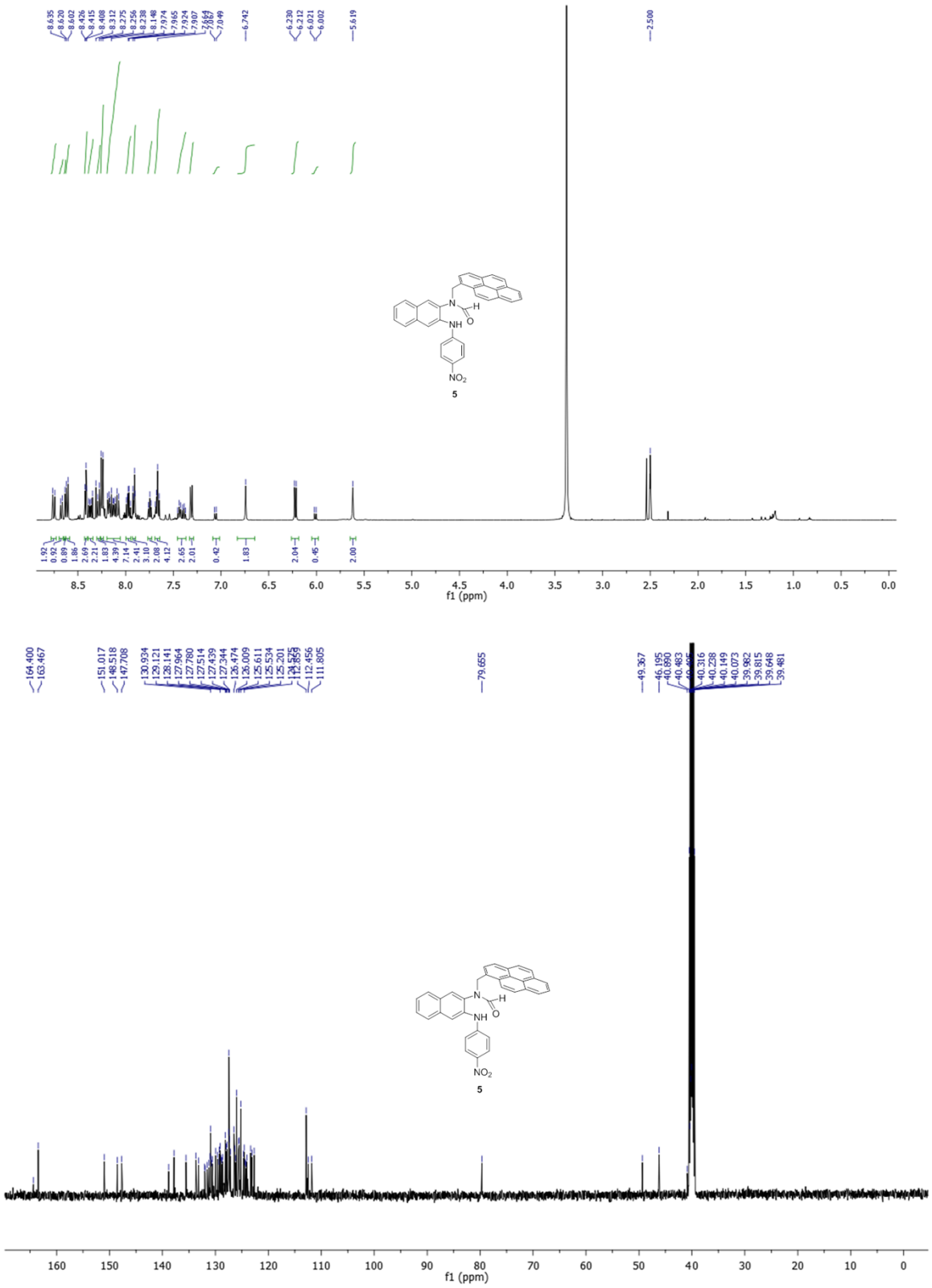
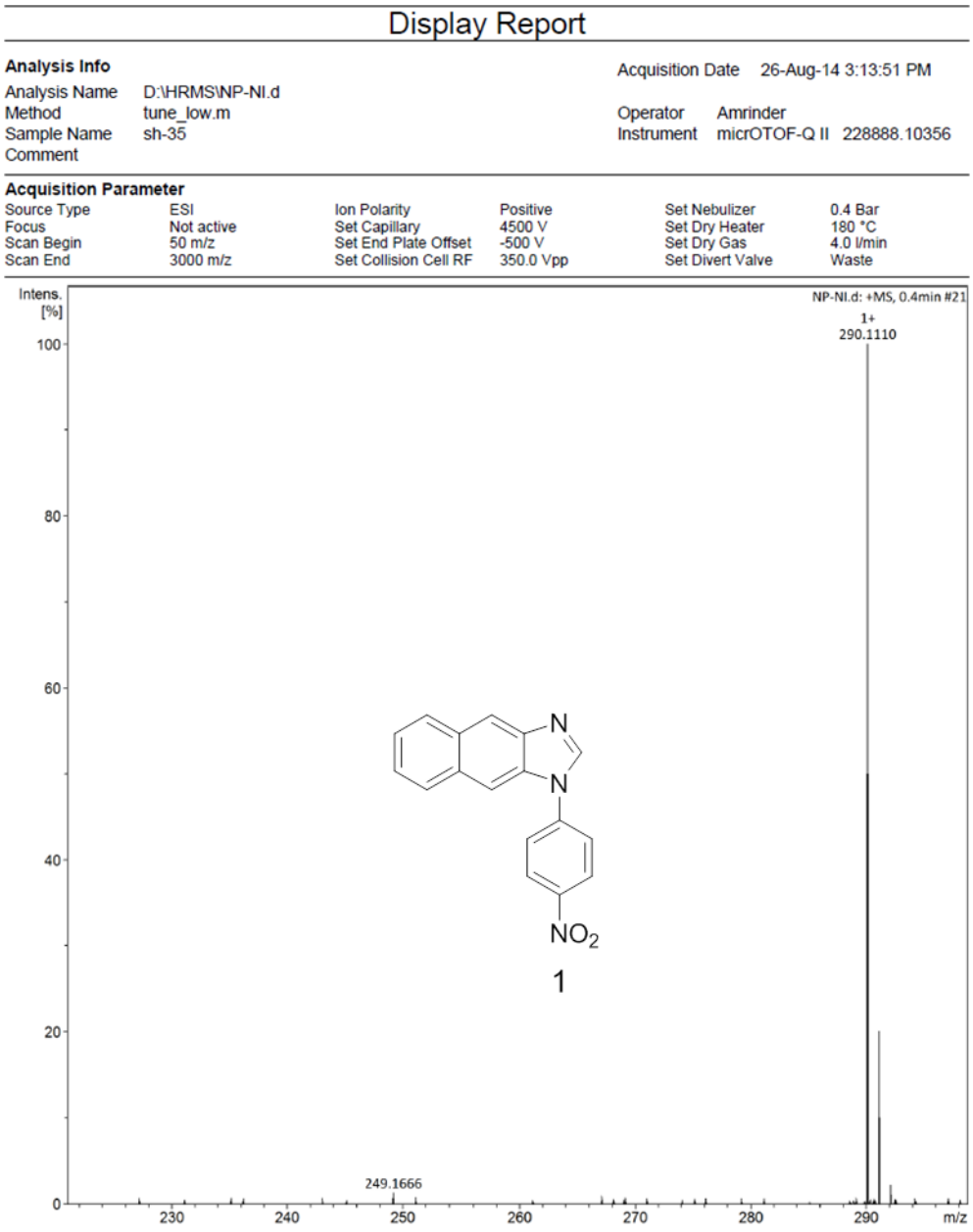


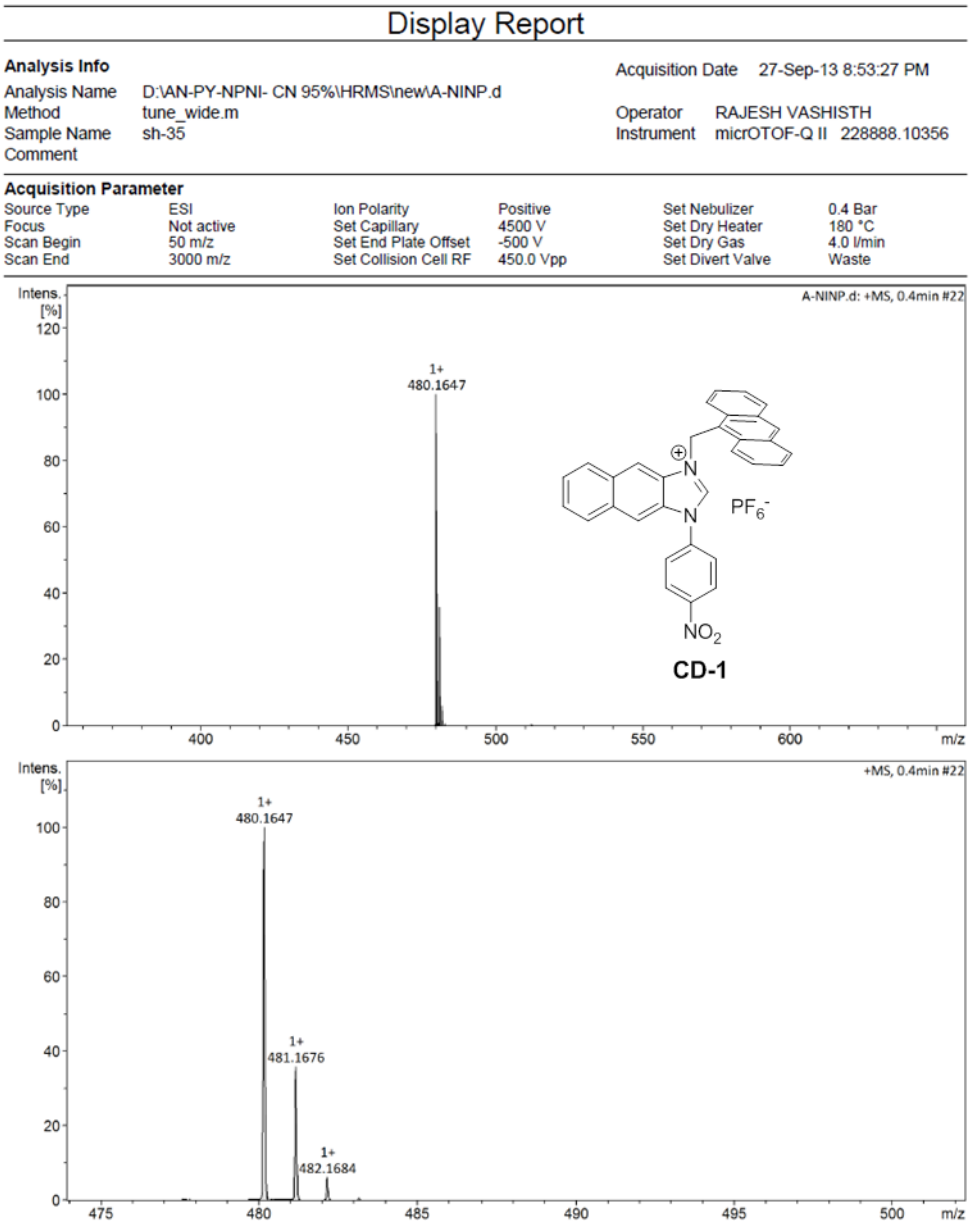
Figure SI 5. ^{1}H and ^{13}C NMR spectra of compound **5**

HRMS spectra of 1, CD-1, CD-2, 4 and 5



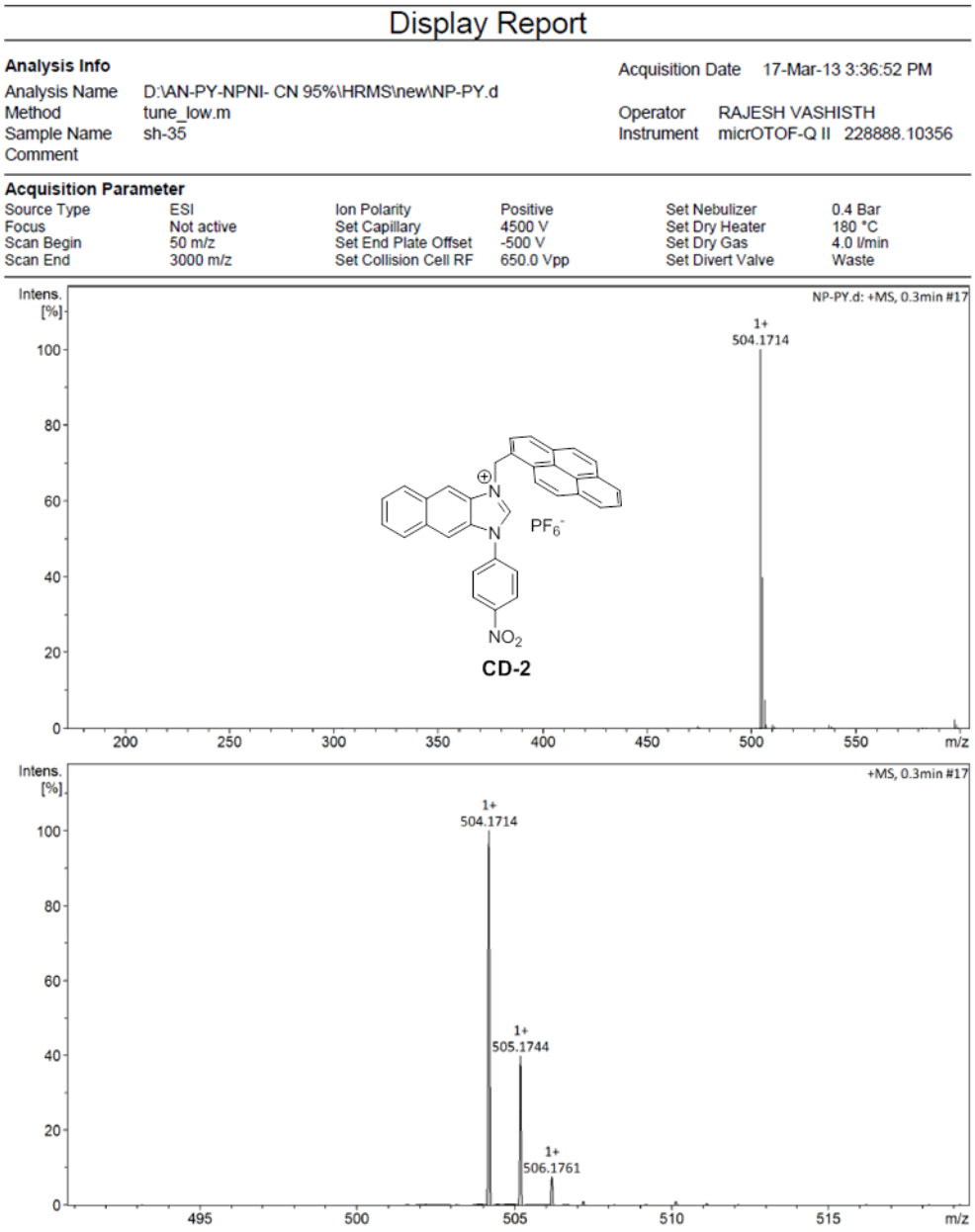
calculated for $C_{17}H_{11}N_3O_2$, m/z = 289.0851 [**1**] ; found 290.1102 [**1** + nH] (100%).

Figure SI 6. HRMS spectrum of **1**



calculated for $C_{32}H_{22}F_6N_3O_2P$, m/z = 480.1707 [CD-**1** - PF_6]$^+$; found 480.1649 [CD-**1** - PF_6]$^+$ (100%).

Figure SI 7. HRMS spectrum of **CD-1**



calculated for $C_{34}H_{22}F_6N_3O_2$, m/z = 504.1707 [CD-**2** - PF_6]$^+$; found 504.1705 [CD-**2** - PF_6]$^+$(100%).

Figure SI 8. HRMS spectrum of **CD-2**

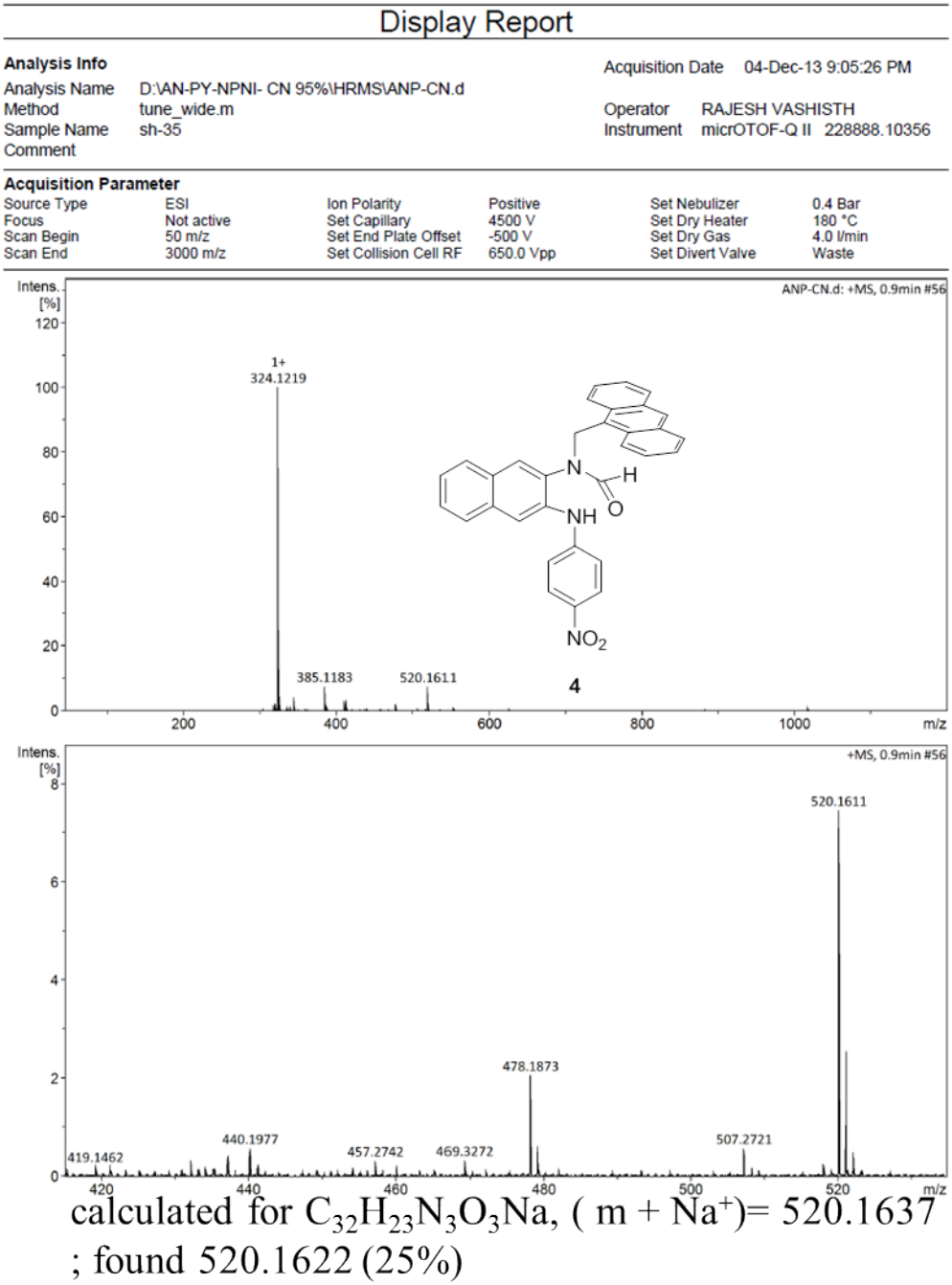
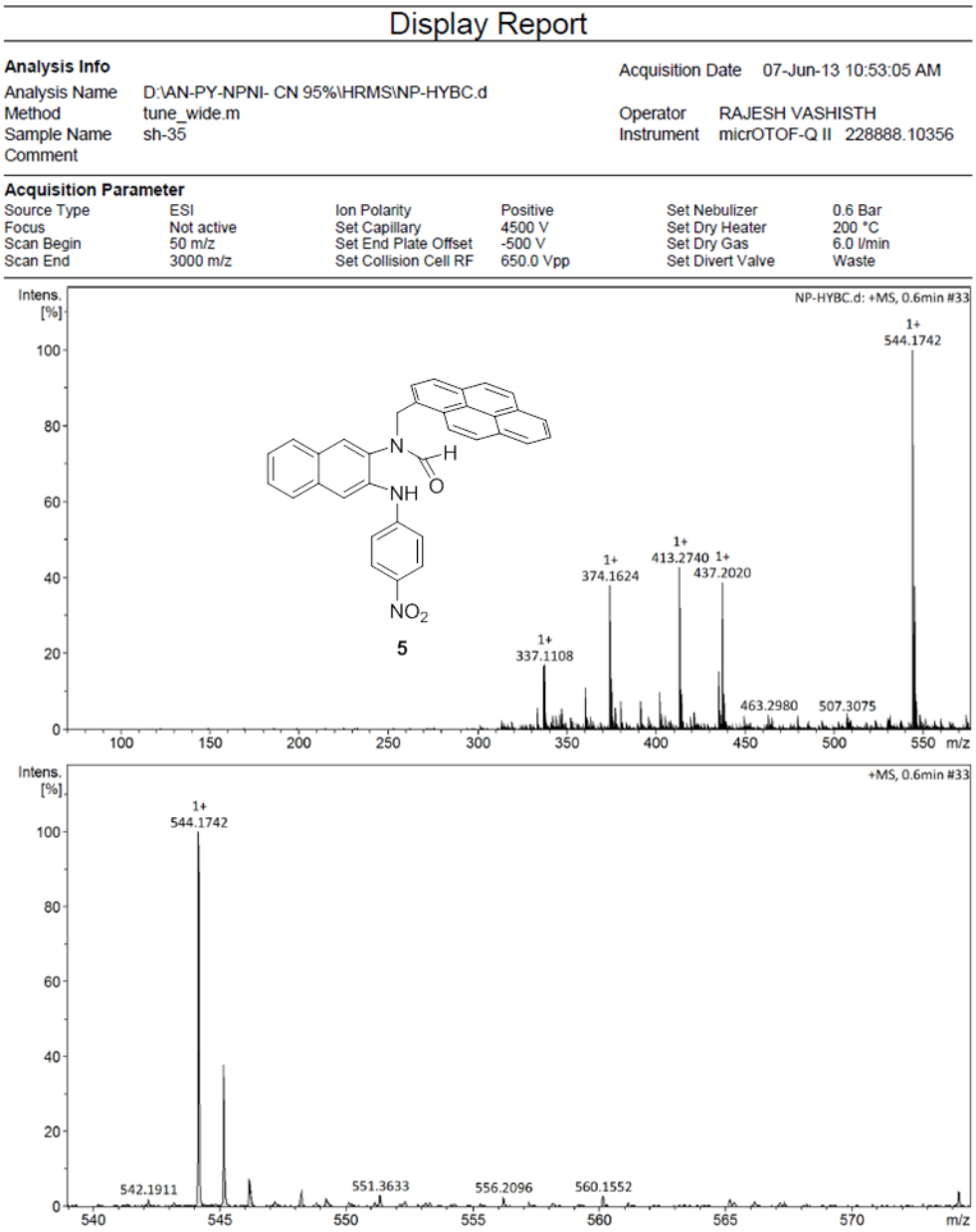


Figure SI 9. HRMS spectrum of compound **4**



calculated for $C_{34}H_{23}N_3O_3Na$, (m + Na^+) = 544.1637 ; found 544.1626 (100%).

Figure SI 10. HRMS spectrum of compound **5**

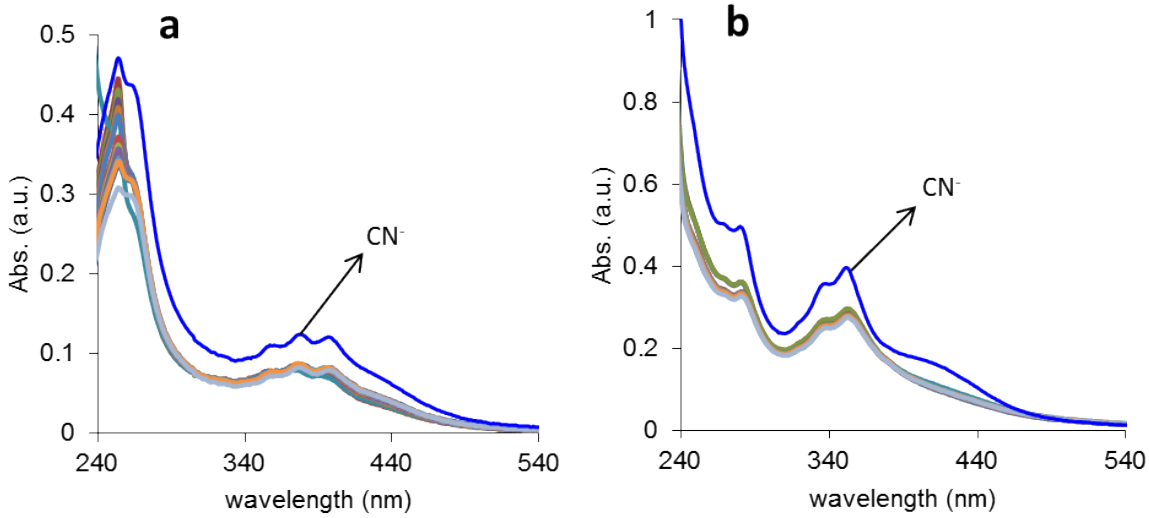


Figure SI 11. (a) Effect of various anions (100 µM) on absorption spectrum of chemodosimeter **CD-1** (5 µM), (b) Effect of various anions (100 µM) on absorption spectrum of chemodosimeter **CD-2** (10 µM) in HEPES buffer - 5% DMSO (pH 7.4).

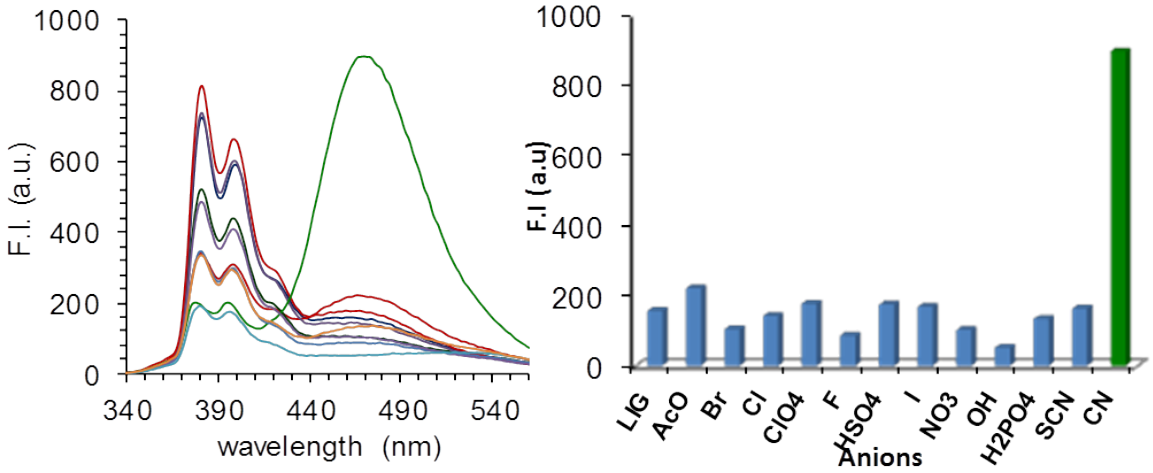


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Figure SI 12. Effect of various anions (100 µM) on emission spectra (λ_{ex} 300 nm) of chemodosimeter **CD-2** (10 µM) in HEPES buffer - 5% DMSO (pH 7.4).

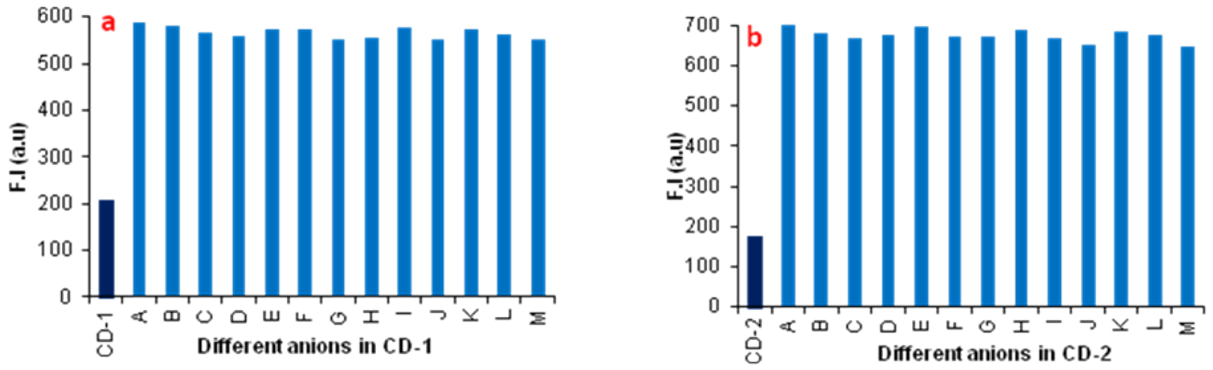

Figure SI 13. Bar diagrams showing the effect of various anions on the emission intensities (λ_{ex} 320 nm) of (a) **CD-1** (5 μM) and (b) **CD-2** (10 μM) in the presence of CN^- and ten thousand times concentration of other anions (100 μM), A (**CD**+CN^-), B (**CD** + AcO^- + CN^-), C (**CD** + F^- + CN^-), D (**CD** + Cl^- + CN^-), E (**CD** + Br^- + CN^-), F (**CD** + I^- + CN^-), G (**CD** + ClO_4^- + CN^-), H (**CD** + $H_2PO_4^-$ + CN^-), I (**CD** + HSO_4^- + CN^-), J (**CD** + SO_4^{2-} + CN^-), K (**CD** + NO_3^- + CN^-), L (**CD** + SCN^- + CN^-) and M (**CD** + OH^- + CN^-) in HEPES buffer - 5% DMSO solution (pH 7.4).

CCDC Numbers

CD-1 CCDC 1042262
Formula: C32 H22 N3 O2 1+,F6 P1 1-,2(C2 H3 N1)
Unit Cell Parameters: a 9.895(3) b 11.505(5) c 14.869(4) P-1

Compound 4 : CCDC 1042263
Formula: C32 H23 N3 O3
Unit Cell Parameters: a 9.816(4) b 11.381(4) c 13.411(6) P-1

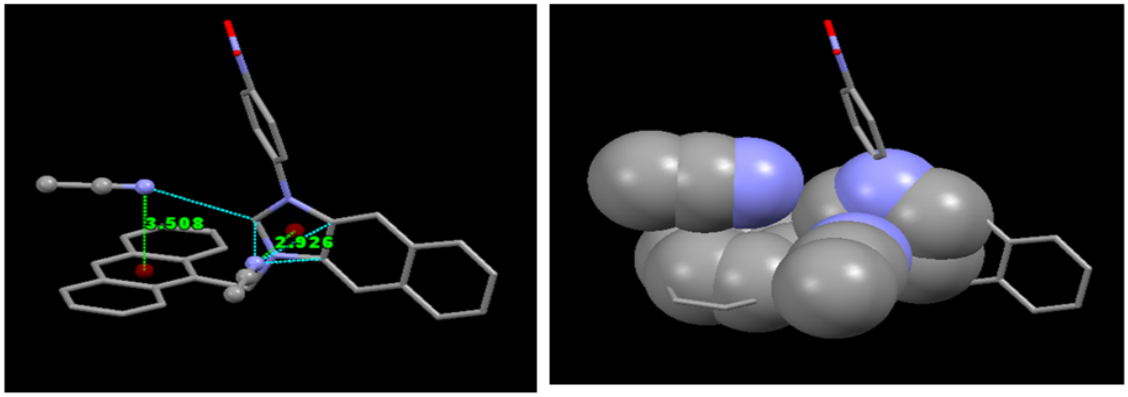

Figure SI 14. Shows lone pair…π interactions of acetonitrile molecules with anthracene and imidazole rings in **CD-1**(a) stick diagram (b) space filled representation.

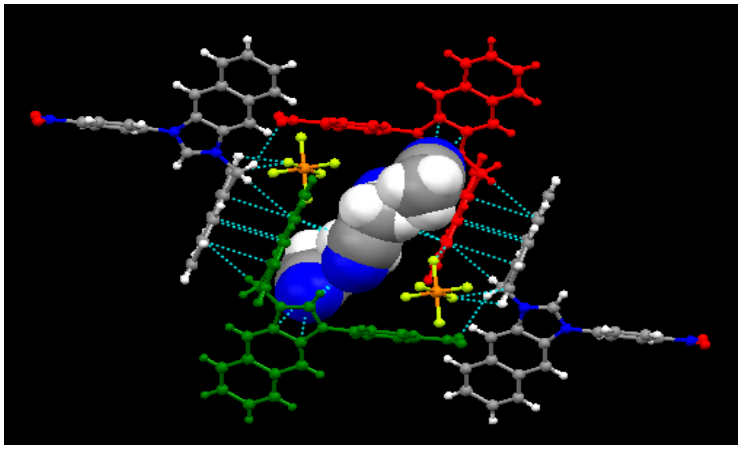

Figure SI 15. The formation of a pseudo-square cavity bound by two centrosymmetric molecules (shown in red and green), the solvent (blue and grey space filled) and anions (yellow and orange balls) held by various non-covalent interactions. π…π interactions between two anthracene rings of two such consecutive dimers form linear chains.

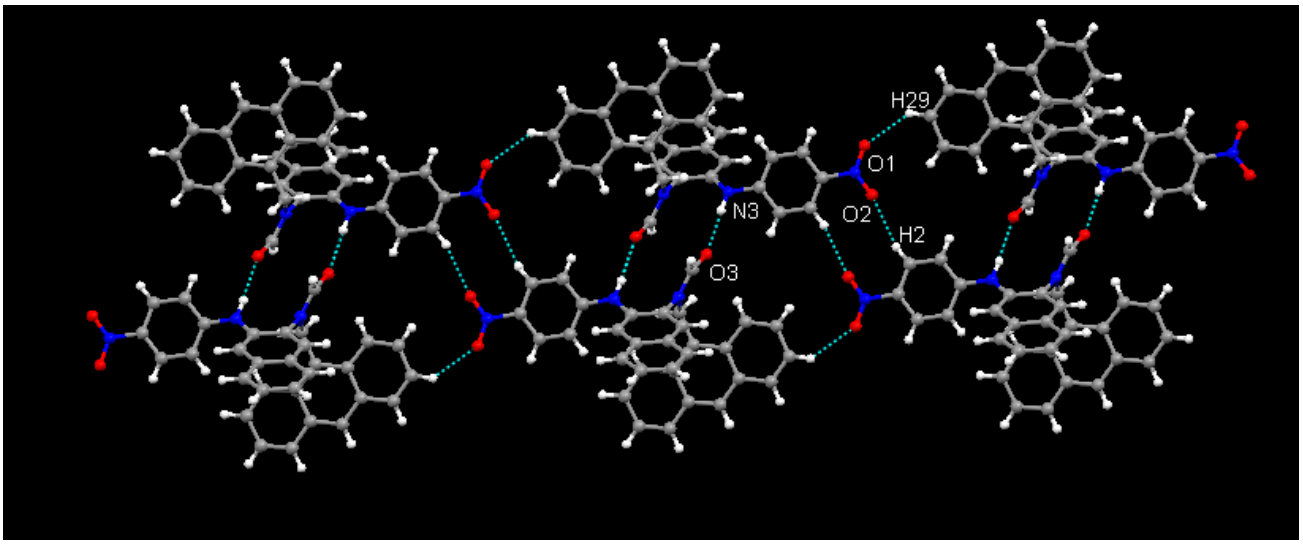

Figure SI 16. Shows the formation of linear H-bonded tapes in compound **4**

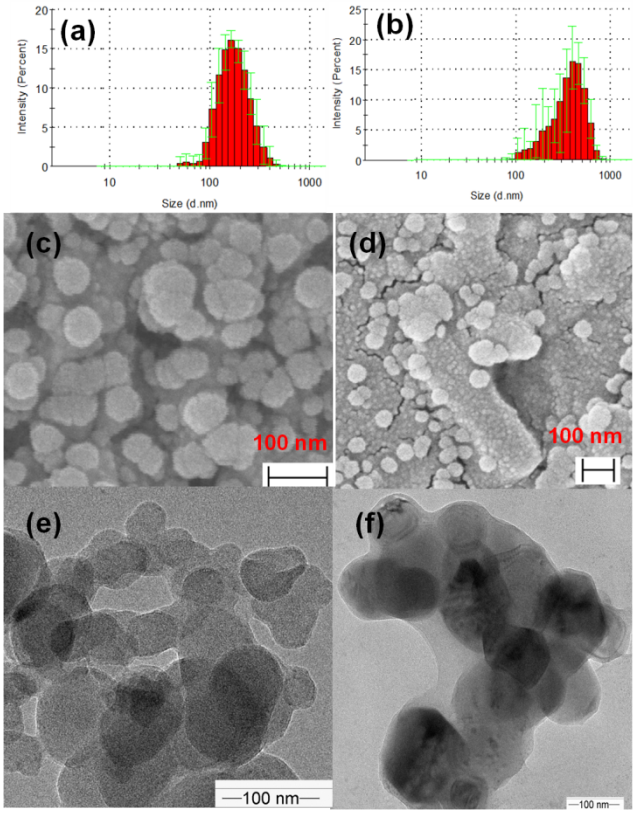

Figure SI 17. DLS (a, b), SEM (c, d) and TEM (e, f) studies of **CD-2** (5 μM, H_2O – DMSO 5%) in the absence (a, c, e) and presence (b, d, f) of CN^-

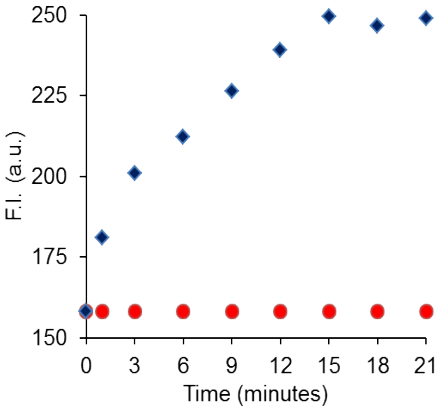

Figure SI 18. Blue diamonds show increase in FI of **CD-1** (5μM) + NaCN (5 nM) solution with time and red circles show no change in FI of **CD-1** alone during this time period.

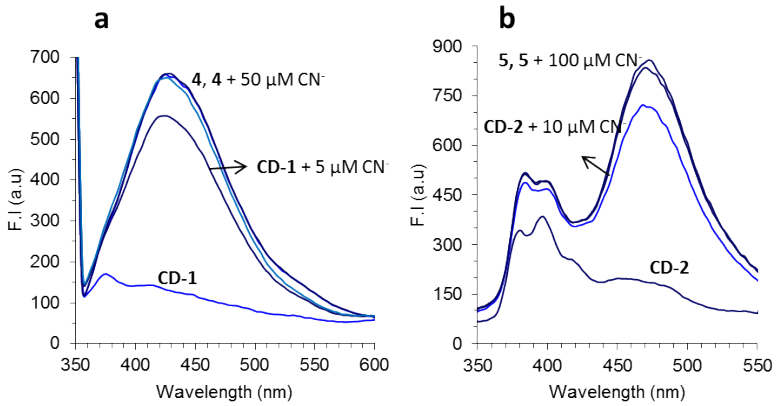

Figure SI 19. Comparison of emission spectra of **(a) CD-1** (5 µM) + CN^- solution with formamide **4** and **(b) CD-2** (10 µM) + CN^- solution with formamide **5**.

Bio-imaging of cyanide ions in live C6 cells

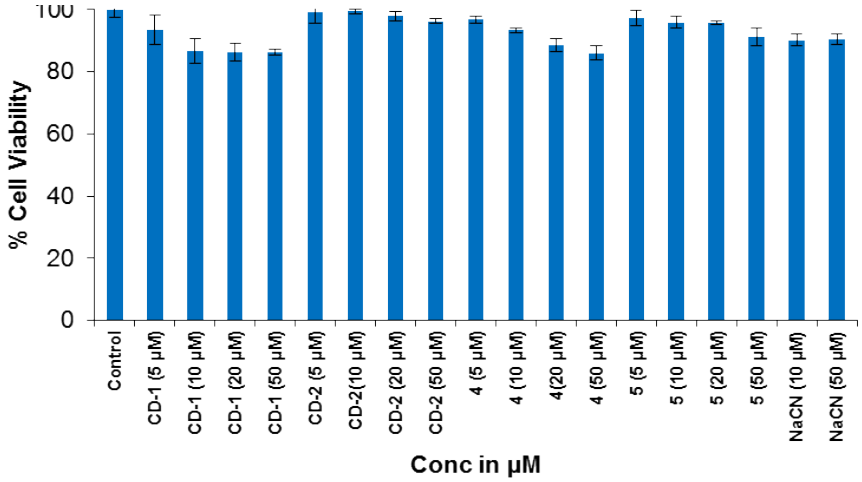

Figure. **SI 20**. Cell viability of C6 glioma cells tested by MTT assay after exposure to 5 µM, 10 µM, 20 µM and 50 µM concentrations of **CD-1** and **CD-2**, and also NaCN (10 µM and 50 µM) for 30 min. C6 cells treated with **CD-1** indicated nearly 86% cell viability while with **CD-2** treatment > 96% C6 cells were viable.

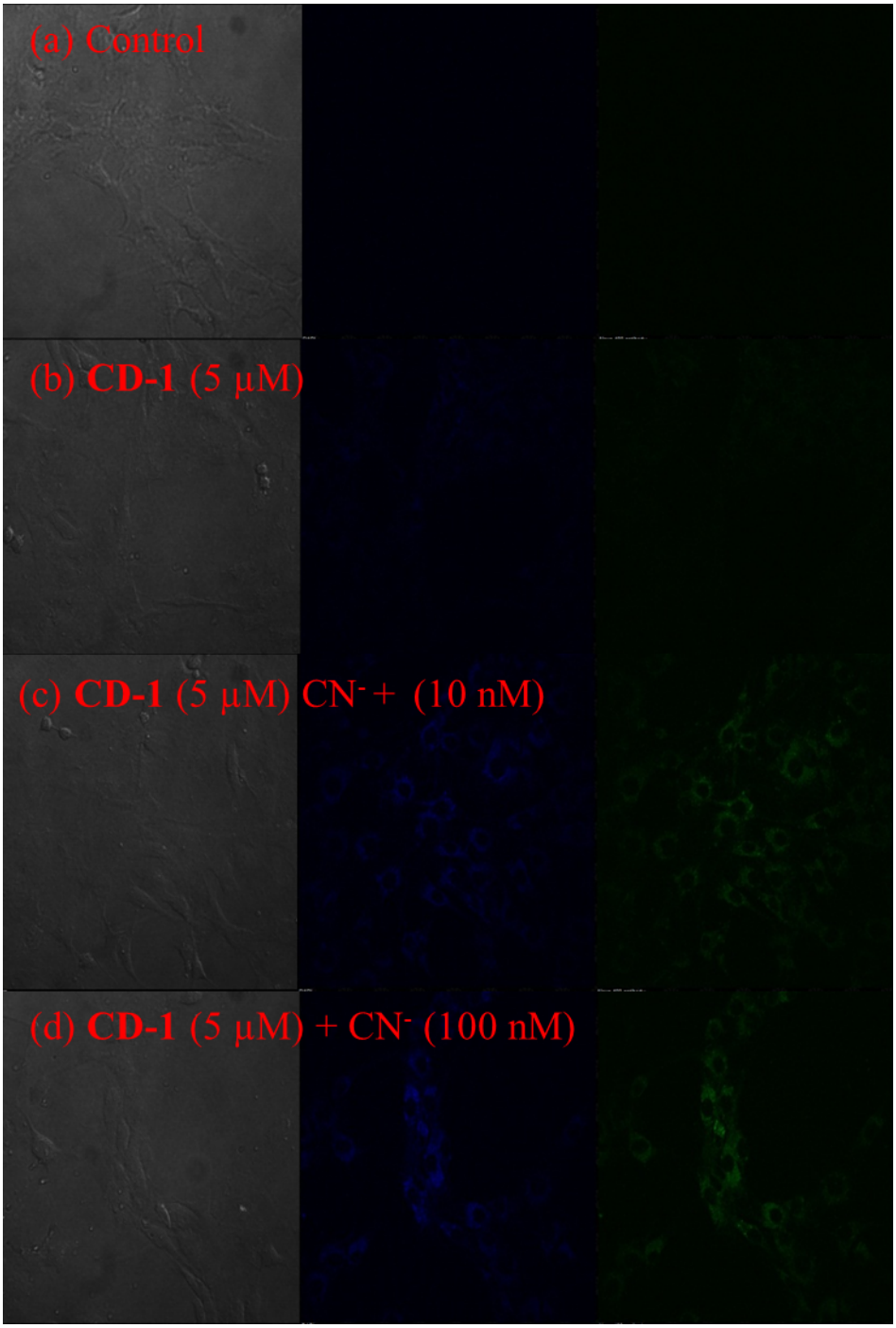

Figure SI 21. Respective images of C6 glioma cells are as brightfield image and under blue and green windows (a) image of untreated C6 glioma cells, (b) fluorescence image of C6 glioma cells treated with chemodosimeter **CD-1**, (c) images of C6 glioma cells incubated with **CD-1** and then with CN^- (10 nM) (d) images of C6 glioma cells incubated with **CD-1** and then with CN^- (100 nM)

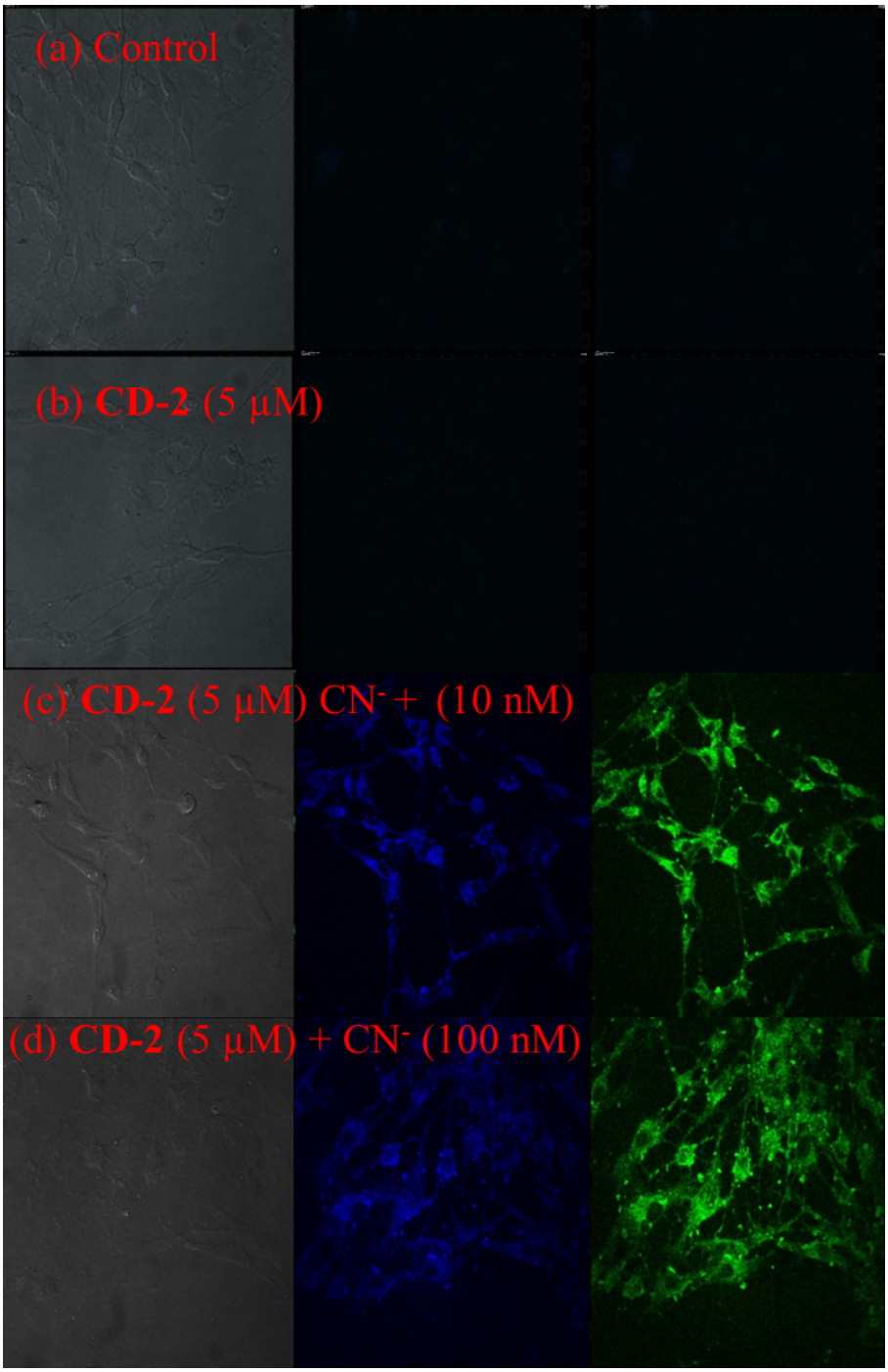

Figure SI 22. Respective images of C6 glioma cells are as brightfield image and under blue and green windows (a) image of untreated C6 glioma cells, (b) fluorescence image of C6 glioma cells treated with chemodosimeter **CD-2**, (c) images of C6 glioma cells incubated with **CD-2** and then with CN^- (10 nM) (d) images of C6 glioma cells incubated with **CD-2** and then with CN^- (100 nM).

Table: List of catalytic chemodosimeters

S.No.	Reference	species	TON/rate
	Present work (first one for anion)	**CN^-**	**70-360/12.64S^{-1}**
1	M. Pal, K. Parasuraman and K. R. Yeleswarapu, *Org. Lett*. 2003, **5**, 349.	Pd^o	NR
2	F. Song, A. L. Garner and K. Koide *J. Am. Chem. Soc*. 2007, **129**, 12354.	Pd^o	NR
3	J. Kovács and A. Mokhir, *Inorg. Chem.* 2008, **47**, 1880;	Cu^{2+}	55
4	D. N. Lee, G. J. Kim and H. J. Kim, *Tetrahedron Lett.*, 2009, **50**, 4766.	Hg^{2+}	2
5	A. L. Garner and K. Koide, *Chem. Commun*., 2009, **86**.	Pd^o, Pt^o	--/ 3.1 h^{-1}
6	A. L. Garner and K. Koide Chem. Commun., 2009, **83**.	Pt^o	--/1200 h^{-1}
7	M. Santra, D. Ryu, A. Chatterjee, S. K. Ko, I. Shin and K. H. Ahn, *Chem. Commun*., 2009, 2115.	Hg^{2+}, CH_3HgCl	2
8	M. H. Kim, H. H. Jang, S. Yi, S. K. Chang and M. S. Han, *Chem. Commun*., 2009, 4838.	Cu^{2+}	NR
9	Q. L. Wang, H. Zhang and Y. B. Jiang, *Tetrahedron Lett.*, 2009, **50**, 29.	Cu^{2+}	20
10	A. L. Garner, F. Song and K. Koide *J. Am. Chem. Soc*. 2009, **131**, 5163.	Pd^o	--/1.8 h^{-1}
11	M. Santra, S. K. Ko, I. Shin and K. H. Ahn, *Chem. Commun*., 2010, **46**, 3964.	Pd^o, Pd^{2+}	NR
12	J. H. Do, H. N. Kim, J. Yoon, J. S. Kim, and H. J. Kim, *Org. Lett*., 2010, **12**, 932.	Au^{3+}	--/3.31x10^{-5} S^{-1} (0.12h^{-1})
13	M. E. Jun and K. H. Ahn, *Org. Lett*., 2010, **12**, 2790.	Pd^o	NR
14	Z. Zhou, N. Li and A. Tong, *Anal. Chim. Acta*., 2011, **702**, 81.	Cu^{2+}	NR

NR = not reported